Building Software With Ease: an Introduction to EasyBuild
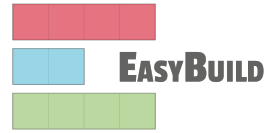
EPICURE webinar, 13 Dec 2024

Kenneth Hoste (HPC-UGent, BE)

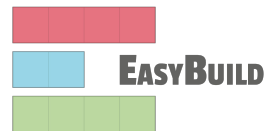**Pedro Santos Neves (Univ. of Groningen, NL)**

Caspar van Leeuwen (SURF, NL)

Agenda

- [14:00-14:10] **What is EasyBuild? + Terminology**

- [14:10-14:20] Installation and configuration of EasyBuild (incl. live demo)

- [14:20-14:30] Basic Usage of EasyBuild (incl. live demo)

- [14:30-14:40] Troubleshooting + sneak peek EasyBuild 5.0 (incl. live demo)

- [14:40-14:55] Adding support for additional software (incl. live demo)

- [14:55-15:00] Advanced topics: hooks & beyond

- [15:00-15:15] Using EasyBuild on top of EESSI (incl. live demo)

- [15:15-15:20] Outlook to EasyBuild 5.0

- [15:20-15:30] Q&A

What is EasyBuild?

- **EasyBuild is a software build and installation framework**

- Strong focus on scientific software, performance, and HPC systems

- Open source (GPLv2), implemented in Python

- Brief history:
  - Created in-house at HPC-UGent in 2008
  - First released publicly in Apr'12 (version 0.5)
  - EasyBuild 1.0.0 released in Nov'12 (during SC12)
  - Worldwide community has grown around it since then!

https://easybuild.io

https://docs.easybuild.io

https://github.com/easybuilders

https://easybuild.io/join-slack

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EasyBuild in a nutshell

- **Tool** to provide a ***consistent and well performing*** scientific software stack

- Uniform interface for installing scientific software on HPC systems

- Saves time by ***automating*** tedious, boring and repetitive tasks

- Can empower scientific researchers to self-manage their software stack

- **A platform for collaboration among HPC sites worldwide**

- Has become an "expert system" for installing scientific software

Key features of EasyBuild (1/2)
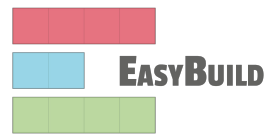
- Supports fully **autonomously** installing (scientific) software, including dependencies, generating environment module files, …

- **No admin privileges are required** (only write permission to installation prefix)

- **Highly configurable**, easy to extend, support for hooks, easy customisation

- Detailed logging, fully transparent via support for "dry runs" and trace mode

- Support for using custom module naming schemes (incl. hierarchical)

Key features of EasyBuild (2/2)

- Integrates with various other tools (Lmod, Singularity, FPM, Slurm, GC3Pie, ...)

- **Actively developed and supported by worldwide community**

- **Frequent stable releases** since 2012 (every 6 - 8 weeks)

- **Comprehensive testing**: unit tests, testing contributions, regression testing

- **Various support channels** (mailing list, Slack, conf calls) + yearly user meetings

Focus points in EasyBuild

Performance

- Strong preference for building software from source

- Software is optimized for the processor architecture of build host (by default)

Reproducibility

- Compiler, libraries, and required dependencies are mostly controlled by EasyBuild

- Fixed software versions for compiler, libraries, (build) dependencies, ...

Community effort

- Development is highly driven by EasyBuild community

- Lots of active contributors, integration with GitHub to facilitate contributions

*Kenneth*

What EasyBuild is _not_

- EasyBuild is **not YABT (Yet Another Build Tool)**

    - It does not try to replace `CMake`, `make`, `pip`, etc.

    - It wraps around those tools and automates installation procedures

- EasyBuild does **not replace traditional Linux package managers** (`yum`, `dnf`, `apt`, …)

    - You should still install some software via OS package manager: OpenSSL, Slurm, etc.

- EasyBuild is **not a magic solution** to all your (software installation) problems

    - You may still run into compiler errors (unless somebody worked around it already)

EasyBuild terminology

- It is important to briefly explain some terminology often used in EasyBuild

- Some concepts are specific to EasyBuild: easyblocks, easyconfigs, ...

- Overloaded terms are clarified: modules, extensions, toolchains, ...
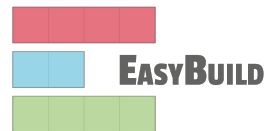
EasyBuild terminology speed run: framework
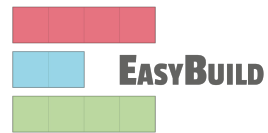
- The EasyBuild framework is the **core of EasyBuild**

- **Collection of Python modules**, organised in packages

- Implements **common functionality** for building and installing software

- Support for applying patches, running commands, generating module files, ...

- Examples: `easybuild.toolchains`, `easybuild.tools`, ...

- Provides `eb` command, but can also be leveraged as a Python library

- GitHub repository: https://github.com/easybuilders/easybuild-framework

EasyBuild terminology speed run: easyblock

- A **Python module** that implements a specific software installation procedure
  - Can be viewed as a "plugin" to the EasyBuild framework

- **Generic easyblocks** for "standard" stuff: `cmake` + `make` + `make install`, Python packages, etc.

- **Software-specific easyblocks** for complex software (OpenFOAM, TensorFlow, WRF, …)

- Installation procedure can be controlled via easyconfig parameters
  - Additional configure options, commands to run before/after build or install command, …
  - Generic easyblock + handful of defined easyconfig parameters is sufficient to install a lot of software

- GitHub repository: https://github.com/easybuilders/easybuild-easyblocks

- Easyblocks do not need to be part of the EasyBuild installation (see `--include-easyblocks`)

EasyBuild terminology speed run: easyconfig file

- "Build recipe"

- Text file that specifies what EasyBuild should install (in Python syntax)

- **Collection of values for easyconfig parameters** (key-value definitions)

- Filename typically ends in '`.eb`'

- Specific filename is expected in some contexts (when resolving dependencies)

  - Should match with values for `name`, `version`, `toolchain`, `versionsuffix`

  - `<name>-<version>-<toolchain><versionsuffix>.eb`

- GitHub repository: https://github.com/easybuilders/easybuild-easyconfigs

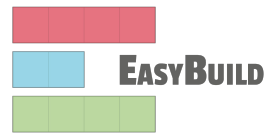# EasyBuild terminology speed run: easystack file

- New concept since EasyBuild v4.3.2 (Dec'20), **experimental feature**

- Concise description for software stack to be installed (in YAML syntax)

- Basically **specifies a set of easyconfig files** (+ associated info)

- Still a work-in-progress, only basic functionality implemented currently

- More info: docs.easybuild.io/easystack-files

EasyBuild terminology speed run: extensions

- **Additional software that can be installed *on top* of other software**

- Common examples: Python packages, Perl modules, R libraries, …

- *Extensions* is the general term we use for this type of software packages

- Can be installed in different ways:
  - As a stand-alone software packages (separate module)
  - In a bundle together with other extensions
  - As an actual extension, to provide a "batteries included" installation

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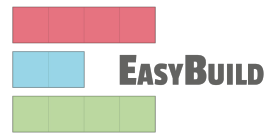# EasyBuild terminology speed run: dependencies

- Software that is **required to build/install or run other software**

- **Build dependencies**: only required when building/installing software (not to use it)

  - Examples: CMake, pip, pkg-config, …

- **Run-time dependencies**: (also) required to use the installed software

  - Examples: Python, Perl, R, …

- **Link-time dependencies**: libraries that are required by software to link to

  - Examples: glibc, OpenBLAS, FFTW, …

- Currently in EasyBuild: no distinction between link-time and run-time dependencies

EasyBuild terminology speed run: toolchains

- **Compiler toolchain: set of compilers + libraries for MPI, BLAS/LAPACK, FFT, …**

- Toolchain component: a part of a toolchain (compiler component, etc.)

- **Full toolchain**: C/C++/Fortran compilers + libraries for MPI, BLAS/LAPACK, FFT

- **Subtoolchain** (partial toolchain): compiler-only, only compiler + MPI, etc.

- **System toolchain**: use compilers (+ libraries) provided by the operating system

- **Common toolchains**: widely used toolchains in EasyBuild community:

  - `foss`: GCC + OpenMPI + (FlexiBLAS +) OpenBLAS + FFTW

  - `intel`: Intel compilers + Intel MPI + Intel MKL

EasyBuild terminology speed run: modules

- Very overloaded term: kernel modules, Python modules, Perl modules …

- In EasyBuild context: "*module*" usually refers to an **environment module file**

  - **Shell-agnostic specification of how to "activate" a software installation**

  - Expressed in Tcl or Lua syntax (scripting languages)

  - Consumed by a modules tool (**Lmod**, Environment Modules, …)

- Other types of modules will be qualified explicitly (Python modules, etc.)

- EasyBuild automatically generates a module file for each installation

Step-wise installation procedure
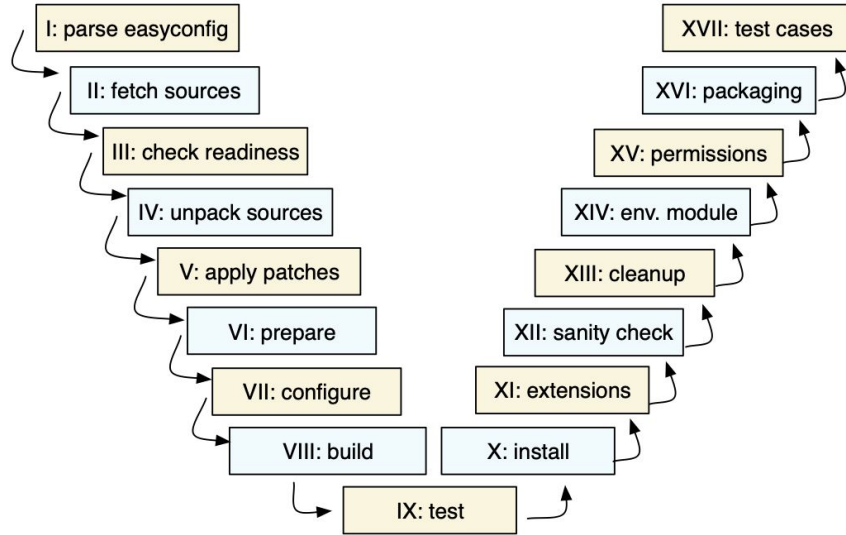
- EasyBuild framework defines step-wise installation procedure, leaves some unimplemented

- Easyblock completes the implementation, override or extends installation steps where needed

- Easyconfig file provides the details (software version, dependencies, toolchain, …)

Bringing all EasyBuild terminology together
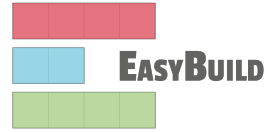
The EasyBuild **framework** leverages **easyblocks** to automatically build and install (scientific) software, potentially including additional **extensions**, using a particular compiler **toolchain**, as specified in **easyconfig files** which each define a set of **easyconfig parameters**.

EasyBuild ensures that the specified **(build) dependencies** are in place, and automatically generates a set of (environment) **modules** that facilitate access to the installed software.
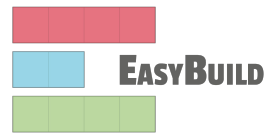
An **easystack** file can be used to specify a collection of software to install with EasyBuild.
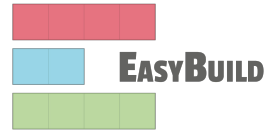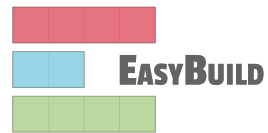
Kenneth

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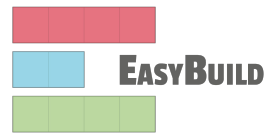*Kenneth*

Installing EasyBuild: requirements

- **Linux** as operating system (CentOS, RHEL, Ubuntu, Debian, SLES, ...)
    - EasyBuild also works on macOS, but support is very basic

- **Python** 2.7 or 3.5+
    - Only Python standard library is required for core functionality of EasyBuild
    - Using Python 3.6+ is highly recommended!

      Python 3.5 won't be supported in EasyBuild 5.0!

- An **environment modules tool** (`module` command)
    - Default is Lua-based Lmod implementation, highly recommended!
    - Tcl-based implementations are also supported

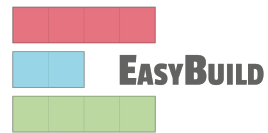*Pedro*

Installing EasyBuild: different options

- Installing EasyBuild using a standard Python installation tool

  - `pip install easybuild`

  - ... or a variant thereof (`pip3 install --user`, using `virtualenv`, etc.)

  - May require additional commands, for example to update environment

- **Installing EasyBuild as a module, with EasyBuild *(recommended!)***

  - 3-step "bootstrap" procedure, via temporary EasyBuild installation using `pip`

- Development setup

  - Clone GitHub repositories:

    `easybuilders/easybuild-{framework,easyblocks,easyconfigs}`

  - Update `$PATH` and `$PYTHONPATH` environment variables

Installing EasyBuild: pip install in Python venv

```
eb-demo $ python3 -m venv eb-env
eb-demo $ source easybuild/bin/activate
(eb-env) eb-demo $ pip install --upgrade pip
…
Successfully installed pip-24.3.1
(eb-env) eb-demo $ pip install easybuild archspec rich
Collecting easybuild
…
Installing collected packages: easybuild-framework, easybuild-easyconfigs,
easybuild-easyblocks, easybuild
Successfully installed easybuild-4.9.4 easybuild-easyblocks-4.9.4
easybuild-easyconfigs-4.9.4 easybuild-framework-4.9.4
…
(eb-env) eb-demo $ eb --version
This is EasyBuild 4.9.4 (framework: 4.9.4, easyblocks: 4.9.4) on host
ip-172-31-13-29.eu-central-1.compute.internal.
```

Pedro

Verifying the EasyBuild installation

- Check EasyBuild version:

  ```
  eb --version
  ```

- Show help output (incl. long list of supported configuration settings)
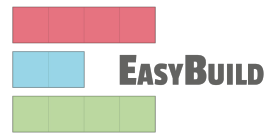
  ```
  eb --help
  ```

- Show the current (default) EasyBuild configuration:

  ```
  eb --show-config
  ```

- Show system information:

  ```
  eb --show-system-info
  ```

Updating EasyBuild (with pip or EasyBuild)

- Updating EasyBuild (in-place) that was installed with pip:

  ```
  pip install --upgrade easybuild
  ```

  (+ additional options like `--user`, or using `pip3`, depending on your setup)

- Use current EasyBuild to install latest EasyBuild release as a module:

  ```
  eb --install-latest-eb-release
  ```

  - This is *not* an in-place update, but a new EasyBuild installation!

 - You need to load (or swap to) the corresponding module afterwards:

    ```
    module load EasyBuild/4.9.4
    ```

Configuring EasyBuild

- EasyBuild should work fine out-of-the-box if you are using Lmod as modules tool

- ... but it will (ab)use `$HOME/.local/easybuild` to install software into, etc.

- **It is *strongly* recommended to configure EasyBuild properly!**

- Main questions you should ask yourself:

    - Where should EasyBuild install software (incl. module files)?

    - Where should auto-downloaded sources be stored?

    - Which filesystem is best suited for software build directories (I/O-intensive)?

Primary configuration settings
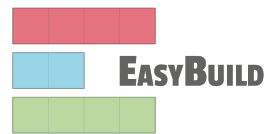
- Most important configuration settings: (strongly recommended to specify the ones in **bold**!)

  - Modules tool + syntax (`modules-tool` + `module-syntax`)

  - **Software + modules installation path** (`installpath`)[*]

  - **Location of software sources "cache"** (`sourcepath`)[*]

  - **Parent directory for software build directories** (`buildpath`)[*]

  - Location of easyconfig files archive (`repositorypath`)[*]

  - Search path for easyconfig files (`robot-paths` + `robot`)

  - Module naming scheme (`module-naming-scheme`)

- Several locations[*] (+ others) can be controlled at once via `prefix` configuration setting

- *Full* list of EasyBuild configuration settings (~270) is available via `eb --help`

Configuration levels

- There are 3 different configuration levels in EasyBuild:
    - **Configuration files**
    - **Environment variables**
    - **Command line options to the eb command**

- Each configuration setting can be specified via each "level" (no exceptions!)

- Hierarchical configuration:
    - Configuration files override default settings
    - Environment variables override configuration files
    - eb command line options override environment variables
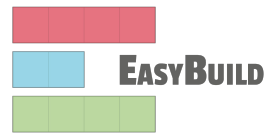
EasyBuild configuration files

- EasyBuild configuration files are in standard INI format (`key=value`)

- EasyBuild considers multiple locations for configuration files:
  - User-level: `$HOME/.config/easybuild/config.cfg` (or via `$XDG_CONFIG_HOME`)
  - System-level: `/etc/easybuild.d/*.cfg` (or via `$XDG_CONFIG_DIRS`)
  - See output of `eb --show-default-configfiles`

- Output produced by `eb --confighelp` is a good starting point

- Typically for "do once and forget" static configuration (like modules tool to use, ...)

- **EasyBuild configuration files and easyconfig files are very different things!**
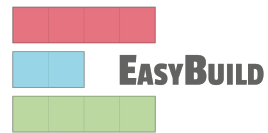
$EASYBUILD_* environment variables

- Very convenient way to configure EasyBuild

- **There is an `$EASYBUILD_*` environment variable for each configuration setting**
  - Use all capital letters
  - Replace every dash (–) character with an underscore (_)
  - Prefix with `EASYBUILD_`
  - Example: `module-syntax` → `$EASYBUILD_MODULE_SYNTAX`

- Common approach: using a shell script or module file to (dynamically) configure EasyBuild
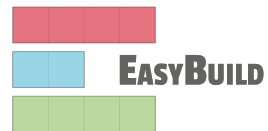
Command line options for eb command

- **Configuration settings specified as command line option always "win"**

- Use double-dash + name of configuration setting, like `--module-syntax`

- Some options have a corresponding shorthand (`eb --robot` == `eb -r`)

- In some cases, only command line option really makes sense (like `eb --version`)

- Typically used to control configuration settings for current EasyBuild session;
  for example: `eb --installpath /tmp/$USER`

Inspecting the current configuration

- It can be difficult to remember how EasyBuild was configured

- Output produced by `eb --show-config` is useful to remind you

- Shows configuration settings that are different from default

- Always shows a couple of key configuration settings

- Also shows on which level each configuration setting was specified

- Full current configuration: `eb --show-full-config`

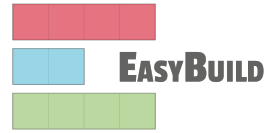# Inspecting the current configuration: example

```
$ cat $HOME/.config/easybuild/config.cfg
[config]
prefix=/apps

$ export EASYBUILD_BUILDPATH=/tmp/$USER/build

$ eb --installpath=/tmp/$USER --show-config
# Current EasyBuild configuration
# (C: command line argument, D: default value,
#  E: environment variable, F: configuration file)
buildpath       (E) = /tmp/example/build
containerpath   (F) = /apps/containers
installpath     (C) = /tmp/example
packagepath     (F) = /apps/packages
prefix          (F) = /apps
repositorypath  (F) = /apps/ebfiles_repo
robot-paths     (D) = /home/example/.local/easybuild/easyconfigs
sourcepath      (F) = /apps/sources
```

Pedro

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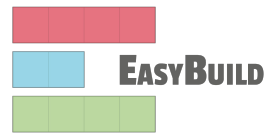*Pedro*

Basic usage of EasyBuild
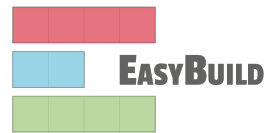
- **Use eb command to run EasyBuild**

- Software to install is usually specified via name(s) of easyconfig file(s), or easystack file

- `--robot` (`-r`) option is required to also install missing dependencies (and toolchain)

- Typical workflow:

  - Find or create easyconfig files to install desired software

  - Inspect easyconfigs, check missing dependencies + planned installation procedure

  - Double check current EasyBuild configuration

  - Instruct EasyBuild to install software (while you enjoy a coffee... or two)

Pedro *https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop/easybuild-basic-usage/* 35

Specifying easyconfigs to use

- The different ways to specify to the `eb` command which easyconfigs to use

  - Specific relative/absolute paths to (directory with) easyconfig files

  - Names of easyconfig files (triggers EasyBuild to search for them)

  - Easystack file to specify a whole stack of software to install (via `eb --easystack`)

- Easyconfig filenames only matter when missing dependencies need to be installed

  - "Robot" mechanism searches based on dependency specs + easyconfig filename

- `eb --search` can be used to quickly search through available easyconfig files

Inspecting easyconfigs via `eb --show-ec`

- To see the contents of an easyconfig file, you can use `eb --show-ec`

- No need to know where it is located, EasyBuild will do that for you!

```
$ eb --show-ec BCFtools-1.18-GCC-12.3.0.eb
easyblock = 'ConfigureMake'

name = 'BCFtools'
version = '1.18'

homepage = 'https://www.htslib.org/'
description = """Samtools is a suite of programs for interacting with high-throughput
sequencing data.
 BCFtools - Reading/writing BCF2/VCF/gVCF files and calling/filtering/summarising SNP and
short indel sequence
 variants"""

toolchain = {'name': 'GCC', 'version': '12.3.0'}
toolchainopts = {'pic': True}
…
```

Checking dependencies via `eb --dry-run`

To check which dependencies are required, you can use `eb --dry-run` (or `eb -D`):

- Provides overview of all dependencies (both installed and missing)

- Including compiler toolchain and build dependencies

```
$ eb BCFtools-1.18-GCC-12.3.0.eb -D
 ...
 * [x] $CFGS/x/XZ/XZ-5.4.2-GCCcore-12.3.0.eb (module: XZ/5.4.2-GCCcore-12.3.0)
 * [x] $CFGS/g/GSL/GSL-2.7-GCC-12.3.0.eb (module: GSL/2.7-GCC-12.3.0)
 * [x] $CFGS/h/HTSlib/HTSlib-1.18-GCC-12.3.0.eb (module: HTSlib/1.18-GCC-12.3.0)
 * [ ] $CFGS/b/BCFtools/BCFtools-1.18-GCC-12.3.0.eb (module:
BCFtools/1.18-GCC-12.3.0)
```

https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop/easybuild-basic-usage/

Checking *missing* dependencies via `eb --missing`

To check which dependencies are still *missing*, use `eb --missing` (or `eb -M`):

- Takes into account available modules, only shows what is still missing

```
$ eb SAMtools-1.18-GCC-12.3.0.eb -M

3 out of 23 required modules missing:

* pkgconf/1.9.5-GCCcore-12.3.0 (pkgconf-1.9.5-GCCcore-12.3.0.eb)

* ncurses/6.4-GCCcore-12.3.0 (ncurses-6.4-GCCcore-12.3.0.eb)

* SAMtools/1.18-GCC-12.3.0 (SAMtools-1.18-GCC-12.3.0.eb)
```

https://tutorial.easybuild.io/2023-eb-eessi-uk-workshop/easybuild-basic-usage/

Inspecting software install procedures

- EasyBuild can quickly unveil how exactly it *would* install an easyconfig file

- Via `eb --extended-dry-run` (or `eb -x`)

- Produces detailed output in a matter of seconds

- Software is not actually installed, all shell commands and file operations are skipped!

- Some guesses and assumptions are made, so it may not be 100% accurate...

- Any errors produced by the easyblock are reported as being ignored

- Very useful to evaluate changes to an easyconfig file or easyblock!

Inspecting software install procedures: example
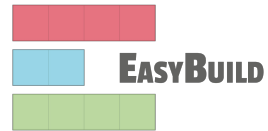
```
$ eb Boost-1.82.0-GCC-12.3.0.eb -x
...

preparing... [DRY RUN]

[prepare_step method]
Defining build environment, based on toolchain (options) and specified dependencies...

Loading toolchain module...

module load GCC/12.3.0

Loading modules for dependencies...
…
```
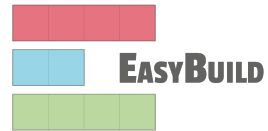
Inspecting software install procedures: example

```
$ eb Boost-1.82.0-GCC-12.3.0.eb -x
...
Defining build environment...
  ...
  export CXX='g++'
  export CXXFLAGS='-O2 -ftree-vectorize -march=native -fno-math-errno -fPIC'
  ...


configuring... [DRY RUN]


[configure_step method]
  running command "./bootstrap.sh --with-toolset=gcc
--prefix=/home/ec2-user/pedro/software/Boost/1.82.0-GCC-12.3.0
--without-libraries=python,mpi"
```
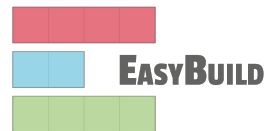
Inspecting software install procedures: example

```
$ eb Boost-1.82.0-GCC-12.3.0.eb -x
...


[sanity_check_step method]

Sanity check paths - file ['files']

  * lib/libboost_system-mt-x64.so

  * lib/libboost_system.so

  * lib/libboost_thread-mt-x64.so

Sanity check paths - (non-empty) directory ['dirs']

  * include/boost

Sanity check commands

  (none)


...
```
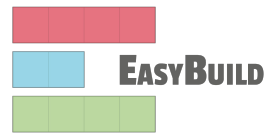
Installing software with EasyBuild

- To install software with EasyBuild, just run the `eb` command:

    - `eb BCFtools-1.18-GCC-12.3.0.eb`

- If any dependencies are still missing, you will need to also use `--robot`:

    - `eb SAMtools-1.18-GCC-12.3.0.eb --robot`

- To see more details while the installation is running, enable trace mode:

    - `eb BCFtools-1.18-GCC-12.3.0.eb --robot --trace`

- To reinstall software, use `eb --rebuild` (or `eb --force`)

Using software installed with EasyBuild

To use the software you installed with EasyBuild, load the corresponding module:

```
# inform modules tool about modules installed with EasyBuild

module use $HOME/easybuild/modules/all

# check for available modules for BCFtools

module avail BCFtools

# load BCFtools module to "activate" the installation

module load BCFtools-1.18-GCC-12.3.0.eb
```
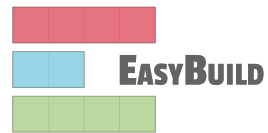
Stacking software installations
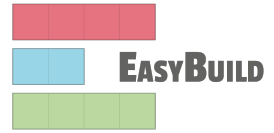
- It's easy to "stack" software installed in different locations

- EasyBuild doesn't care much where software is installed

- As long as the required modules are available to load, it can pick them up

- End users can easily manage a software stack on top of what's installed centrally!

```
module use /easybuild/modules/all

eb --installpath $HOME/easybuild my-software.eb
```

Agenda

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- [14:20-14:30] Basic Usage of EasyBuild (incl. live demo)

- [14:30-14:40] **Troubleshooting + sneak peek EasyBuild 5.0 (incl. live demo)**

- [14:40-14:55] Adding support for additional software (incl. live demo)

- [14:55-15:00] Advanced topics: hooks & beyond

- [15:00-15:15] Using EasyBuild on top of EESSI (incl. live demo)

- [15:15-15:20] Outlook to EasyBuild 5.0

- [15:20-15:30] Q&A

Kenneth

Troubleshooting failing installations

- Sometimes stuff still goes wrong…

- Being able to troubleshoot a failing installation is a useful/necessary skill

- Problems that occur include (but are not limited to):
  - Missing source files
  - Missing dependencies (perhaps overlooked required dependencies)
  - Failing shell commands (non-zero exit status)
  - Running out of memory or storage space
  - Compiler errors (or crashes)

- EasyBuild keeps a thorough log for each installation which is very helpful

Troubleshooting: error messages

- When EasyBuild detects that something went wrong, it produces an error

- Very often due to a shell command that produced a non-zero exit code...

- Sometimes the problem is clear directly from the error message:

```
== building...
== FAILED: Installation ended unsuccessfully (build directory:
/tmp/build/example/1.0/GCC-11.2.0):
build failed (first 300 chars): cmd "make" exited with exit code 2 and output:
/usr/bin/g++ -O2 -ftree-vectorize -march=native -std=c++14 -c -o core.o core.cpp
g++: error: unrecognized command line option '-std=c++14' (took 1 sec)
```

- In some cases, the error message itself does not reveal the problem...
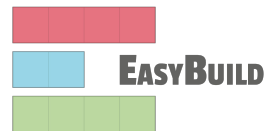
Troubleshooting: log files

- EasyBuild keeps track of the installation in a detailed log file

- During the installation, it is stored in a temporary directory:

  ```
  $ eb example.eb
  == Temporary log file in case of crash /tmp/eb-r503td0j/easybuild-17flov9v.log
  ...
  ```

- Includes executed shell commands and output, build environment, etc.

- More detailed log file when debug mode is enabled (`debug` configuration setting)

- There is a log file per EasyBuild session, and one per performed installation

- **When an installation completes successfully,
  the log file is copied to a subdirectory of the software installation directory**

Troubleshooting: navigating log files

- **EasyBuild log files are well structured, and fairly easy to search through**

- Example log message, showing prefix ("== "), timestamp, source location, log level:

  ```
  == 2022-05-25 13:11:19,968 run.py:222 INFO running cmd:  make -j 9
  ```
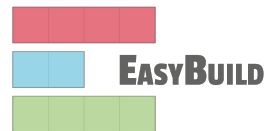
- Different steps of installation procedure are clearly marked:

  ```
  == 2022-05-25 13:11:48,817 example INFO Starting sanity check step
  ```

- To find actual problem for a failing shell command, look for patterns like:
  - ERROR
  - Error 1
  - error:
  - failure
  - not found
  - No such file or directory
  - Segmentation fault

Troubleshooting: inspecting the build directory

- EasyBuild leaves the build directory in place when the installation failed
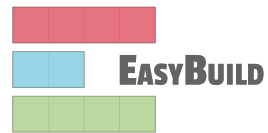
  ```
  == FAILED: Installation ended unsuccessfully (build directory:
  /tmp/build/example/1.0/GCC-11.2.0): build failed ...
  ```

- Can be useful to inspect the contents of the build directory for debugging

- For example:

  - Check `config.log` when `configure` command failed

  - Check `CMakeFiles/CMakeError.log` when `cmake` command failed (good luck...)

Sneak peek at troubleshooting with EasyBuild v5.0

- **EasyBuild v5.0 will make troubleshooting failing installations significantly easier**

- When a shell command run by EasyBuild fails:

  - The problem will be reported in a more user-friendly way

  - You can quickly inspect (only) the output of that command

  - A script is generated to start an **interactive session** to debug "in context":
    in the correct working directory + prepared build environment

- Made possible by switching to new `run_shell_cmd` function

- ETA for EasyBuild v5.0: in the coming ~~months~~ weeks…

Running development version of EasyBuild v5.0

One way to already experiment with the development version of EasyBuild 5.0

is by installing the 5.0.x branches of the main EasyBuild GitHub repositories:

```
python3 -m venv eb5-venv

source eb5-venv/bin/activate

for x in framework easyblocks easyconfigs; do

  pip install https://github.com/easybuilders/easybuild-$x/archive/5.0.x.tar.gz

done
```

Note: at some point in the coming months weeks we will collapse each `5.0.x` branch
into the corresponding `develop` branch, and remove the `5.0.x` branches!

Improved error reporting in EasyBuild v5.0

EasyBuild 5.0 produces clearer error messages when a shell command failed:

```
ERROR: Shell command failed!
    full command            ->  make  -j 8 LDFLAGS='-lfast'
    exit code               ->  2
    called from             ->  'build_step' function in /.../easyblocks/generic/configuremake.py (line 357)
    working directory       ->  /tmp/ec2-user/kenneth/easybuild/build/BCFtools/1.18/GCC-12.3.0/bcftools-1.18
    output (stdout + stderr)  ->  /tmp/eb-i61vle8x/run-shell-cmd-output/make-1ynysa6f/out.txt
    interactive shell script  ->  /tmp/eb-i61vle8x/run-shell-cmd-output/make-1ynysa6f/cmd.sh
```

- Colors to draw attention to the most important parts of the error message

- File with (only) command output + path to build directory are easy to find

- Auto-generated `cmd.sh` script starts **interactive subshell** to debug the problem in the correct build environment!
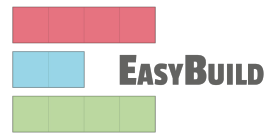
This is powered by the new `run_shell_cmd` function that EasyBuild uses to run shell commands,
which took a lot of effort, partially because all ~240 easyblocks has to be updated to use `run_shell_cmd`.

Agenda
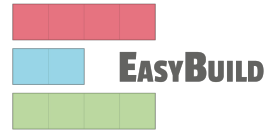
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Adding support for additional software
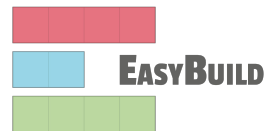
- Every installation performed by EasyBuild requires an easyconfig file

- Easyconfig files can be:

    - Included with EasyBuild itself (or obtained elsewhere)

    - Derived from an existing easyconfig (manually or automatic)

    - Created from scratch

- Most easyconfigs leverage a generic easyblock

- Sometimes using a custom software-specific easyblock makes sense...
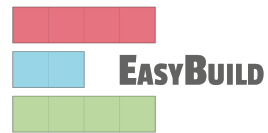
Easyblocks vs easyconfigs

- When can you get away with using an easyconfig leveraging a generic easyblock?

- When is a software-specific easyblock really required?

- Easyblocks are *"implement once and forget"*

- Easyconfig files leveraging a generic easyblock can become too complicated (subjective)

- Reasons to consider implementing a custom easyblock:
  - 'critical' values for easyconfig parameters required to make installation succeed
  - custom (configure) options related to toolchain or included dependencies
  - interactive commands that need to be run
  - having to create or adjust specific (configuration) files
  - 'hackish' usage of a generic easyblock
  - complex or very non-standard installation procedure

Writing easyconfig files
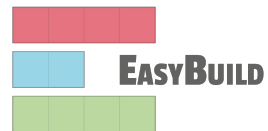
- Collection of easyconfig parameter definitions (Python syntax),

  collectively specify what to install

- Some easyconfig parameters are **mandatory**, and must always be defined:

  `name`, `version`, `homepage`, `description`, `toolchain`

- Commonly used easyconfig parameters (but strictly speaking not required):
  - `easyblock` (by default derived from software name)
  - `versionsuffix`
  - `source_urls`, `sources`, `patches`, `checksums`
  - `dependencies`, `builddependencies`
  - `preconfigopts`, `configopts`, `prebuildopts`, `buildopts`, `preinstallopts`, `installopts`
  - `sanity_check_paths`, `sanity_check_commands`

Generating tweaked easyconfig files

- Trivial changes to existing easyconfig files can be done automatically

- Bumping software version: `eb example-1.0.eb --try-software-version 1.1`

- Changing toolchain (version): `eb example.eb --try-toolchain GCC,12.3.0`

- Changing specific easyconfig parameters (limited): `eb --try-amend ...`

- Note the "try" aspect: additional changes may be required to make installation work

- EasyBuild does save the so generated easyconfig files in the `easybuild` subdirectory of the software installation directory and in the easyconfig archive.

Copying easyconfig files

- Small but useful feature: copy specified easyconfig file via `eb --copy-ec`

- Avoids the need to locate the file first via `eb --search`

- Typically used to create a new easyconfig using existing one as starting point

- Example:

  ```
  $ eb --copy-ec BCFtools-1.18-GCC-12.3.0.eb BCFtools.eb
  ...
  BCFtools-1.18-GCC-12.3.0.eb copied to BCFtools.eb
  ```

Exercise on creating easyconfig file from scratch

- Step-wise example + exercise of creating an easyconfig file from scratch

- For fictitious software packages: `eb-tutorial` + `py-eb-tutorial`

- Sources available at

  https://github.com/easybuilders/easybuild-tutorial/tree/main/docs/files

- **Great exercise to work through these yourself!**
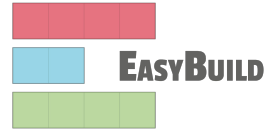
```
name = 'eb-tutorial'

version = '1.0.1'

homepage = 'https://easybuilders.github.io/easybuild-tutorial'

description = "EasyBuild tutorial example"
```

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- [14:55-15:00] **Advanced topics: hooks & beyond**

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- [15:20-15:30] Q&A

The EasyBuild community

EasyBuild User Meeting 2020 (Barcelona)
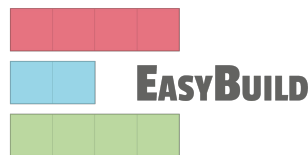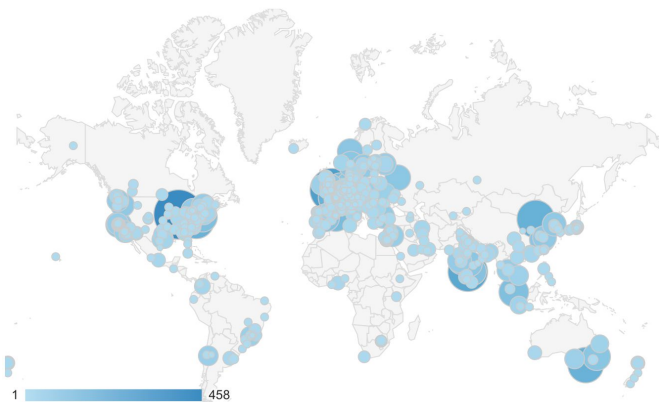
- Documentation is read all over the world

- HPC sites, consortia, and companies

- Slack: >700 members, ~180 active members

  per week, 311k messages

- Regular online conf calls… and we even meet in person sometimes!

Contributing to EasyBuild

There are several ways to contribute to EasyBuild, including:

- Providing feedback (positive or negative)

- Reporting bugs

- Joining the discussions (mailing list, Slack, conf calls)

- Sharing suggestions/ideas for enhancements & additional features

- Contributing easyconfigs, enhancing easyblocks,

  adding support for new software, implementing additional features, ...

- Extending & enhancing documentation

GitHub integration features
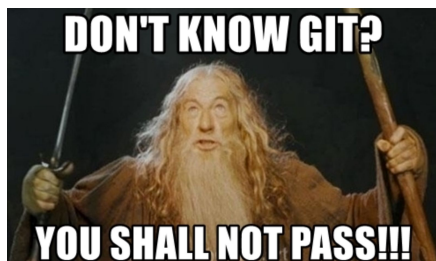
- EasyBuild has strong integration with GitHub, which facilitates contributions

- Some additional Python packages required for this: GitPython, keyring

- Also requires some additional configuration, incl. providing a GitHub token

- **Enables creating, updating, reviewing pull requests using eb command!**

- Makes testing contributions very easy: ~2,500 easyconfig pull requests per year!

- Extensively documented:

  docs.easybuild.io/integration-with-github

Opening a pull request in 1, ~~2~~, ~~3~~

```
$ mv sklearn.eb scikit-learn-1.4.2-gfbf-2023a.eb
$ mv scikit-learn*.eb easybuild/easyconfigs/s/scikit-learn
$ git checkout develop && git pull upstream develop
$ git checkout -b scikit_learn_142_gfbf_2023a
$ git add easybuild/easyconfigs/s/scikit-learn
$ git commit -m "{data}[gfbf/2023a] scikit-learn v1.4.2"
$ git push origin scikit_learn_142_gfbf_2023a
```

+ log into GitHub to actually open the pull request (clickety, clickety...)

one single `eb` command

no git commands

no GitHub interaction

metadata is automatically derived from easyconfig

saves a lot of time!

eb --new-pr sklearn.eb

Kenneth

EASYBUILD

Customizing EasyBuild via Hooks

- Hooks allow you to customize EasyBuild easily and consistently

- Set of Python functions that are automatically picked up by EasyBuild

- Can be used to "hook" custom code into specific installation steps

- Make EasyBuild use your hooks via `hooks` configuration option

- Examples:
  - Inject or tweak configuration options

  - Change toolchain definitions

  - Custom checks to ensure that site policies are taken into account

- Extensively documented: docs.easybuild.io/hooks

Hooks: examples

- EUM'22 talk by Alex: Building a heterogeneous MPI stack with EasyBuild

  https://easybuild.io/eum22/#eb-mpi

- `contrib/hooks` subdirectory in easybuild-framework GitHub repository:

  https://github.com/easybuilders/easybuild-framework/tree/develop/contrib/hooks

Hooks: examples

Ensure that software is installed with a specific license group:

```python
def parse_hook(self, *args, **kwargs):

    if self.name == 'example':

        # use correct license group for software 'example'

        self['group'] = 'licensed_users_example'
```

Implementing Easyblocks

- An easyblock may be required for more complex software installations

- This requires some Python skills, and familiarity with EasyBuild framework

- A software-specific easyblock can derived from a generic easyblock

- Focus is usually on configure/build/installs steps of installation procedure

- See also https://docs.easybuild.io/implementing-easyblocks

Submitting Installations as Slurm Jobs

- EasyBuild can *distribute* the installation of a software stack as jobs on a cluster

- Slurm is the most commonly used job backend that EasyBuild can use

- `export EASYBUILD_JOB_BACKEND=Slurm`

- Use "`eb … --job --robot`" to submit software installations

  to be performed with EasyBuild as Slurm jobs

- See also https://docs.easybuild.io/submitting-jobs
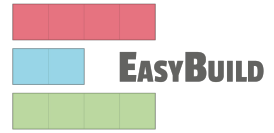
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Installing something with a lot of dependencies…

- For example, PyTorch…

```
$ eb --missing PyTorch-bundle-2.1.2-foss-2023a.eb

144 out of 164 required modules missing:

* pkgconf/1.9.5-GCCcore-12.3.0 (pkgconf-1.9.5-GCCcore-12.3.0.eb)

* UnZip/6.0-GCCcore-12.3.0 (UnZip-6.0-GCCcore-12.3.0.eb)

* expat/2.5.0-GCCcore-12.3.0 (expat-2.5.0-GCCcore-12.3.0.eb)

...

* sympy/1.12-gfbf-2023a (sympy-1.12-gfbf-2023a.eb)

* PyTorch/2.1.2-foss-2023a (PyTorch-2.1.2-foss-2023a.eb)

* PyTorch-bundle/2.1.2-foss-2023a (PyTorch-bundle-2.1.2-foss-2023a.eb)
```

- That's going to take forever…

What is EESSI?
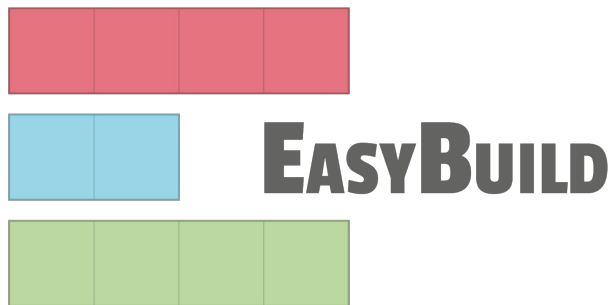
EESSI in a nutshell

- *European Environment for Scientific Software Installations (EESSI)*

- **Shared repository of (optimized!) scientific software _installations_**

- Avoid duplicate work across (HPC) sites by collaborating on a shared software stack

- Uniform way of providing software to users, regardless of the system they use!

- Should work on any Linux OS (+ WSL, and macOS[*]) and system architecture
  - From laptops and personal workstations to HPC clusters and cloud
  - Support for different CPUs, interconnects, GPUs, etc.

- **Focus on performance, automation, testing, collaboration**

https://www.eessi.io/docs/

EESSI
EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

[*]through Lima
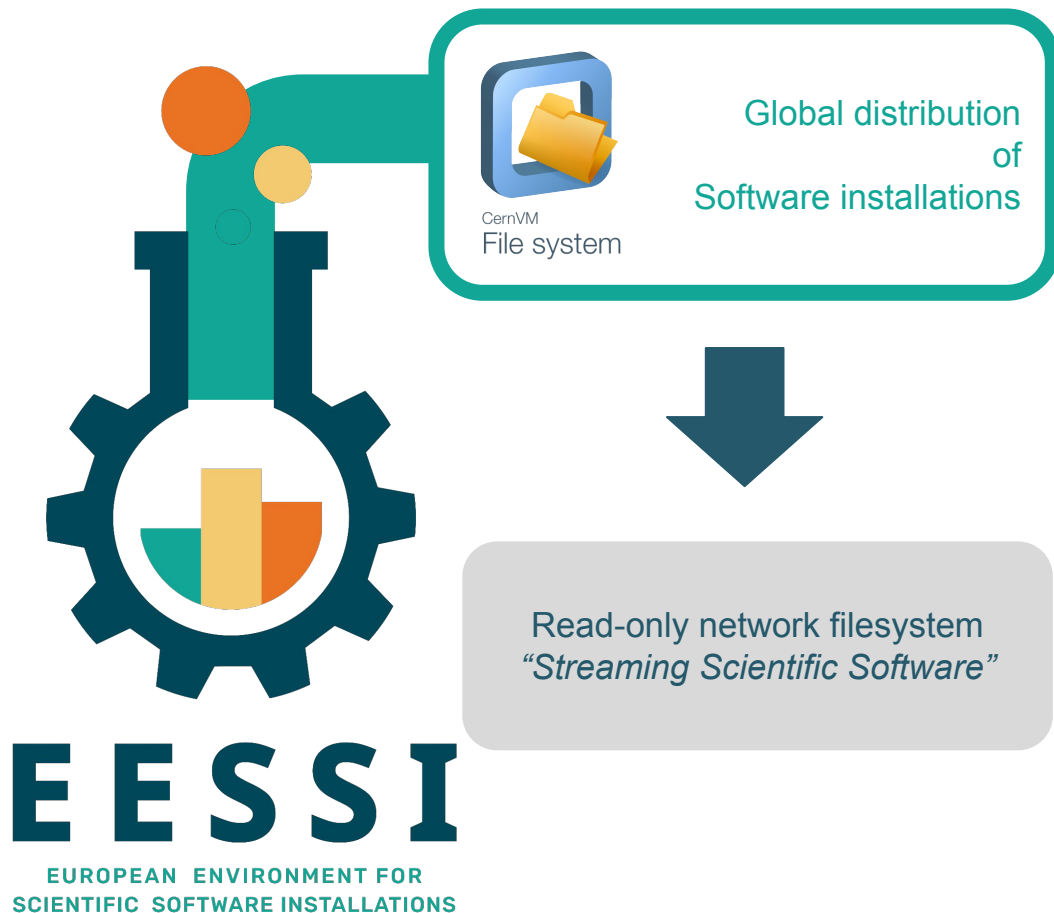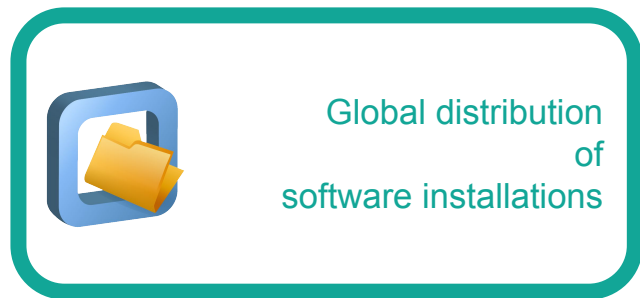
Caspar

EESSI ingredients

CernVM
File system

Global distribution
of
Software installations

Read-only network filesystem
"Streaming Scientific Software"

EESSI

EUROPEAN ENVIRONMENT FOR
SCIENTIFIC SOFTWARE INSTALLATIONS

EESSI ingredients

Abstraction from the host OS

Similar to container images
"Containers without the Containing"

Global distribution of software installations

EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS
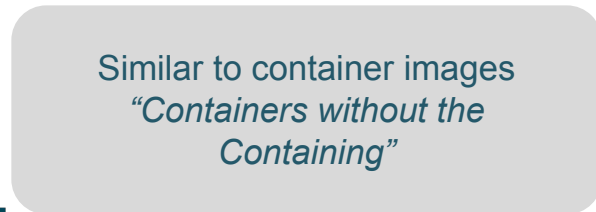
EESSI ingredients

Abstraction from the host OS
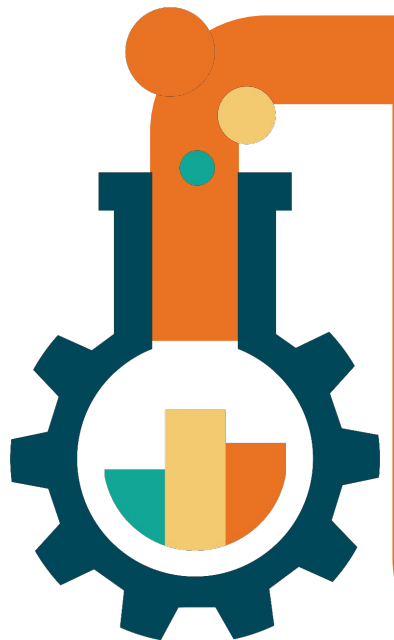
Global distribution of software installations

Optimized software Installations for specific CPU microarchitectures

Intuitive user interface: module avail, module load, …
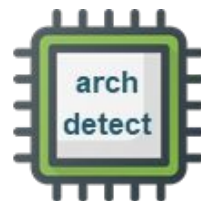
Automatic selection of Best suited part of Software stack for CPU microarchitectures

EESSI

EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Using EESSI

- Here, we'll assume EESSI is already installed. If not, follow instructions on eessi.io/docs/getting_access/native_installation/

- Set up EESSI environment by loading the module

```
$ ls /cvmfs/software.eessi.io
host_injections   init   README.eessi   versions

$ module unuse $MODULEPATH

$ module use /cvmfs/software.eessi.io/init/modules

$ module load EESSI/2023.06
EESSI/2023.06 loaded successfully...

$ module avail

...
```

Caspar

EESSI-extend: building on top of EESSI with EasyBuild

- EESSI provides base installations

- We can install on top of the EESSI software stack with EasyBuild

```
$ module load EESSI-extend/2023.06-easybuild

-- Using /tmp/$USER as a temporary working directory for installations, you can override this
by setting the environment variable WORKING_DIR and reloading the module (e.g., /dev/shm is a
common option)

Configuring for use of EESSI_USER_INSTALL under /home/ec2-user/eessi

-- To create installations for EESSI, you _must_ have write permissions to
/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4

-- You may wish to configure a sources directory for EasyBuild (for example, via setting the
environment variable EASYBUILD_SOURCEPATH) to allow you to reuse existing sources for
packages.
```

EESSI-extend: building on top of EESSI with EasyBuild

- EESSI provides base installations

- We can install on top of the EESSI software stack with EasyBuild

```
$ eb --missing PyTorch-bundle-2.1.2-foss-2023a.eb

11 out of 138 required modules missing:



* parameterized/0.9.0-GCCcore-12.3.0 (parameterized-0.9.0-GCCcore-12.3.0.eb)

* Scalene/1.5.26-GCCcore-12.3.0 (Scalene-1.5.26-GCCcore-12.3.0.eb)

...

* PyTorch-bundle/2.1.2-foss-2023a (PyTorch-bundle-2.1.2-foss-2023a.eb)
```

- Much more feasible!

EESSI-extend: how does it work?

- Configures EasyBuild very similar to how main EESSI software stack is built

```
$ eb --show-config
...
filter-deps          (E) = Autoconf, Automake, Autotools, binutils, bzip2, DBus, flex,
gettext, gperf, help2man, intltool, libreadline, libtool, M4, makeinfo, ncurses, util-linux,
XZ, zlib
filter-env-vars      (E) = LD_LIBRARY_PATH
hooks                (E) =
/cvmfs/software.eessi.io/versions/2023.06/init/easybuild/eb_hooks.py
...
installpath          (E) =
/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4
...
rpath                (E) = True
...
sysroot              (E) = /cvmfs/software.eessi.io/versions/2023.06/compat/linux/x86_64
```

Caspar

EESSI-extend: how does it work?

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...
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gettext, gperf, help2man, intltool, libreadline, libtool, M4, makeinfo, ncurses, util-linux,
xz, zlib
filter-env-vars   (E) = LD_LIBRARY_PATH
hooks             (E) =
/cvmfs/software.eessi.io/versions/2023.06/init/easybuild/eb_hooks.py
...
installpath       (E) =
/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4
...
rpath             (E) = True
...
sysroot           (E) = /cvmfs/software.eessi.io/versions/2023.06/compat/linux/x86_64
```

These deps are provided by Gentoo-prefix

EESSI-extend: how does it work?

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filter-env-vars     (E) = LD_LIBRARY_PATH
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/cvmfs/software.eessi.io/versions/2023.06/init/easybuild/eb_hooks.py
...
installpath         (E) =
/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4
...
rpath               (E) = True
...
sysroot             (E) = /cvmfs/software.eessi.io/versions/2023.06/compat/linux/x86_64
```

Libraries are found at runtime by setting RPATH instead of
LD_LIBRARY_PATH (avoids host OS executables from using libs from EESSI)

EESSI-extend: how does it work?

- Configures EasyBuild very similar to how main EESSI software stack is built

```
$ eb --show-config
...
filter-deps          (E) = Autoconf, Automake, Autotools, binutils, bzip2, DBus, flex,
gettext, gperf, help2man, intltool, libreadline, libtool, M4, makeinfo, ncurses, util-linux,
XZ, zlib
filter-env-vars      (E) = LD_LIBRARY_PATH
hooks                (E) =
/cvmfs/software.eessi.io/versions/2023.06/init/easybuild/eb_hooks.py
...
installpath          (E) =
/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4
...
rpath                (E) = True
...
sysroot              (E) = /cvmfs/software.eessi.io/versions/2023.06/compat/linux/x86_64
```

A set of EasyBuild hooks that are used to fix issues (e.g. software X doesn't build on ARM with vectorization => disable vectorization)

EESSI-extend: how does it work?

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```
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...
filter-deps          (E) = Autoconf, Automake, Autotools, binutils, bzip2, DBus, flex,
gettext, gperf, help2man, intltool, libreadline, libtool, M4, makeinfo, ncurses, util-linux,
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filter-env-vars      (E) = LD_LIBRARY_PATH
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/cvmfs/software.eessi.io/versions/2023.06/init/easybuild/eb_hooks.py
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/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4
...
rpath                (E) = True
...
sysroot              (E) = /cvmfs/software.eessi.io/versions/2023.06/compat/linux/x86_64
```

Installpath contains architecture + micro-architecture, as detected by architect. Mimics EESSI directory structure.

EESSI-extend: how does it work?

- Configures EasyBuild very similar to how main EESSI software stack is built

```
$ eb --show-config
...
filter-deps         (E) = Autoconf, Automake, Autotools, binutils, bzip2, DBus, flex,
gettext, gperf, help2man, intltool, libreadline, libtool, M4, makeinfo, ncurses, util-linux,
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filter-env-vars     (E) = LD_LIBRARY_PATH
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/cvmfs/software.eessi.io/versions/2023.06/init/easybuild/eb_hooks.py
...
installpath         (E) =
/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4
...
rpath               (E) = True
...
sysroot             (E) = /cvmfs/software.eessi.io/versions/2023.06/compat/linux/x86_64
```

Tells EasyBuild that the OS against which it has to build (Gentoo-prefix)
resides in this prefix

Environment variables that influence EESSI-extend

WARNING: you need to set the environment variables before loading EESSI-extend

- `$EESSI_CVMFS_INSTALL`

    - to install in the main EESSI prefix (/cvmfs/software.eessi.io/versions/...)

    - for CVMFS admins of the EESSI repository only

    - Umask: 022.

    - Example: `EESSI_CVMFS_INSTALL=1`

- `$EESSI_SITE_INSTALL`

    - install dir will be $EESSI_SITE_SOFTWARE_PATH (default: /cvmfs/software.eessi.io/host_injections/...)

    - for HPC support staff building a local software environment (for end-users) on top of EESSI

    - Umask: 022.

    - Example: `EESSI_SITE_INSTALL=1`

Environment variables that influence EESSI-extend

- `$EESSI_PROJECT_INSTALL`

    - install in `$EESSI_PROJECT_INSTALL/versions/<eessi_version>/software/<os>/$EESSI_SOFTWARE_SUBDIR`

    - for project groups (i.e. end users) to build a common software stack in e.g. a project space

    - Umask: 002. Group-writeable-installdir: true. Set-gid-bit: true. Sticky bit: false.

    - Example: EESSI_PROJECT_INSTALL=/my/project/dir (dir has to exist!)

- `$EESSI_USER_INSTALL` *(default)*

    - install in `$EESSI_USER_INSTALL/versions/<eessi_version>/software/<os>/$EESSI_SOFTWARE_SUBDIR`

    - for individual end-users, to build additional software in their homedir

    - Umask: 077. Sticky bit: true.

    - Example: EESSI_USER_INSTALL=$HOME/my/prefix (dir has to exist!)

EESSI-extend: demo time!

- Let's (re)install PyTorch-bundle-2.1.2-foss-2023a.eb

```
$ eb PyTorch-bundle-2.1.2-foss-2023a.eb --robot

...

== COMPLETED: Installation ended successfully (took 14 secs)

== Results of the build can be found in the log file(s)
/home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4/software/PyTorch-bundle/
2.1.2-foss-2023a/easybuild/easybuild-PyTorch-bundle-2.1.2-20241209.133133.log.bz2


== Build succeeded for 1 out of 1

...
$ module av PyTorch-bundle/2.1.2-foss-2023a


------ /home/ec2-user/eessi/versions/2023.06/software/linux/x86_64/amd/zen4/modules/all
-------
   PyTorch-bundle/2.1.2-foss-2023a (D)
...
```

Caspar

EESSI-extend, final remarks:

- If you don't set any of the `EESSI_*_INSTALL` environment vars, `EESSI-extend` defaults to `EESSI_USER_INSTALL=$HOME/eessi`

- `EESSI-extend` installs and optimizes for the current host

  - Installpath based on current host architecture

  - Default EasyBuild optimization is used: `--optarch=None`, meaning native optimization

  - If your login node has different architecture from your batch nodes, install on a batch node

  - On a heterogenous cluster, you will *probably* want to install everything once per architecture in your cluster

- Modules installed with `EESSI-extend` are only visible *after* loading `EESSI-extend` again

https://www.eessi.io/docs/using_eessi/building_on_eessi/

Paper (open access): https://doi.org/10.1002/spe.3075

Website: https://www.eessi.io

Join our Slack channel
https://join.slack.com/t/eessi-hpc/shared_invite/zt-1wqy0t8g
6-PZJTg3Hjjm5Fm3XEOkzECg

Documentation: https://eessi.github.io/docs

GitHub: https://github.com/eessi

Twitter: @eessi_hpc

YouTube channel (brand new!)

Bi-monthly online meetings (first Thu odd months, 2pm CEST)

Outlook to EasyBuild v5.0

- **EasyBuild v5.0 should get released in the coming ~~months~~ weeks...**

- Being prepared in the `5.0.x` branches, soon to be collapsed in `develop` branches

- Includes **breaking changes** + **changed defaults** for some configuration options

- **Requires Python 3.6+** (3.9+ recommended), Python 2.7 no longer supported

- **Requires Lmod version >= 8.0** or Environment Modules version >= 4.3.0

- Enabled by default: **trace** output, **RPATH** linking, `depends_on` in Lua modules, using `pip`, ...

- Framework + easyblocks migrated to new `run_shell_cmd` function → **better error reporting**

- Deprecated functionality: `run_cmd`, `run_cmd_qa`, using Environment Modules version < 4.0, ...

- There will be **no more releases of EasyBuild 4.x** once EasyBuild 5.0 is released!

- All changes will be clearly documented – **Early testing & feedback is very welcome!**

Questions?

- Website: https://easybuild.io

- Documentation: https://docs.easybuild.io

- Tutorials: https://tutorial.easybuild.io

- **Yearly EasyBuild User Meeting: https://easybuild.io/eum (25-27 March 2025 in Jülich, Germany)**

- Getting help:

    - Mailing list: https://lists.ugent.be/wws/subscribe/easybuild

    - Slack: https://easybuild.slack.com - https://easybuild.io/join-slack

    - Bi-weekly conference calls: https://github.com/easybuilders/easybuild/wiki/Conference-calls